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Synthesis, cytotoxic activity and DNA-binding properties of copper(II) complexes with terpyridine

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Abstract

Mononuclear copper(II) complexes with 2,2':6',2''-terpyridine (terpy), [Cu(terpy)(ClO_4)$_2$(H_2O)] (**1**) and [Cu(terpy)$_2$](CF_3SO_3)$_2$·2H_2O (**2**), were synthesized and structurally characterized by UV-vis and IR spectroscopy, ESI mass spectrometry and single-crystal X-ray diffraction analysis. *In vitro* study of cytotoxicity of the complexes demonstrated good antiproliferative properties in the case of human non-small cell lung cancer (A549), as well as in lung fibroblast (MRC5) cell line. Copper(II) complexes with terpy showed significant ability to interact with the high molecular weight double stranded DNA, without induction of DNA damage. On the other side, they caused nicking of plasmid DNA without presence of co-oxidant, indicating moderate nucleolytic activity. Circular dichroism spectra confirmed intercalation of the complexes to double-stranded DNA. Molecular docking studies also indicated strong binding affinity of the complexes with DNA revealing that two forms of **1** (**1a** and **1b** with and without coordinated perchlorate ion, respectively) and **2** bind to the major groove of DNA.

Keywords: Copper(II) complexes, Terpyridine, Cytotoxicity, DNA interaction, Docking studies

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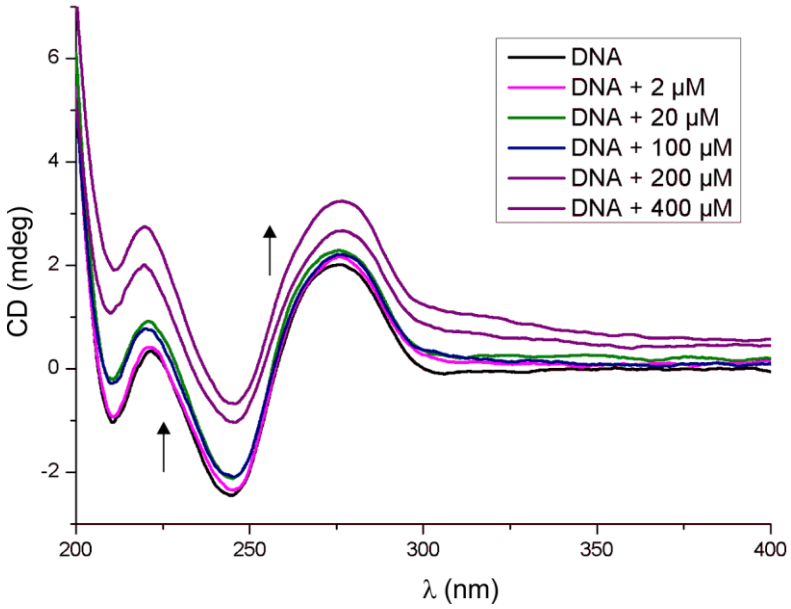

Fig. S1. CD spectra of DNA in the absence and presence of complex **2** (2 - 400 µM) in Tris-HCl buffer (pH 7.4).